Inelastic X-ray Scattering Study of Mott Insulators

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Introduction: Inelastic x-ray scattering (IXS) is the ideal/natural probe of dynamic charge fluctuations at intermediate and high energies. The discovery of a remnant fermisurface and d-wave like high-energy gap in cuprate insulator (ARPES study by F. Ronning et al., (1998)) instigates our interest to study the k-resolved unoccupied upper Hubbard band (UHB) in parent high Tc cuprate.

Methods and Materials: This IXS experiment was performed at NSLS/X-21 near Cu K-edge of cuprate insulator Ca2CuO2Cl2 in order to get enhancement of electronic excitations (with an overall resolution better than 450 meV).

Results: Our x-ray scattering study shows that the Mott excitations (near 2.5 eV) are highly dispersive along <110> and are higher in energy but along <100> they are less dispersive and somewhat lower in energy. These results from X-21 reveal the anisotropy of full Mott gap (figure-1) in insulating cuprates (Hasan et.al., (2000)).

Conclusions: In this experiment we demonstrate the utility and power of IXS in probing the electronic structure of complex insulators. The details of the q-dependence of charge-transfer (effective Mott) excitations would determine important issues like the significance of long-range hopping and the lowest energy state of the upper Hubbard band. Such new fundamental electronic information may lead to better understanding of superconductivity in these classes of oxides.

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References: M.Z. Hasan, E.D. Isaacs, Z.X. Shen et.al., Science 288 , 1811 (2000); F. Ronning et al., Science 282, 2067 (1998)

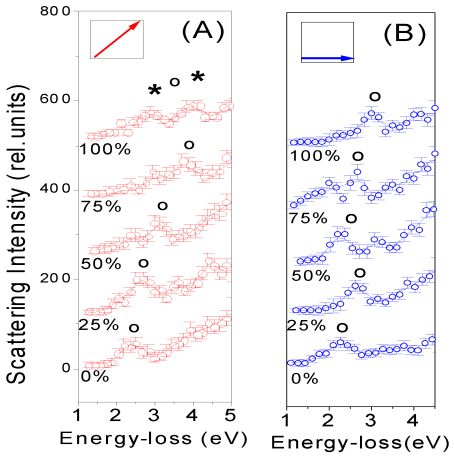

Figure 1. IXS spectra of Ca2CuO2Cl2 along two high symmetry directions. Directions are shown in the inset of each panel.